

Glossary of Terms Used in Medicinal Chemistry  
(IUPAC Recommendations 1998)

## A to H

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### Active transport\*

**Active transport** is the carriage of a solute across a biological membrane from low to high concentration that requires the expenditure of (metabolic) energy.

### Address-message concept

**Address-message concept** refers to compounds in which part of the molecule is required for binding (address) and part for the biological action (message).

### ADME

Abbreviation for **Absorption**, **Distribution**, **Metabolism**, **Excretion**. (See also **Pharmacokinetics**; **Drug disposition**).

### Affinity

**Affinity** is the tendency of a molecule to associate with another. The **affinity** of a **drug** is its ability to bind to its biological target (**receptor**, **enzyme**, transport system, etc.) For pharmacological **receptors** it can be thought of as the frequency with which the **drug**, when brought into the proximity of a **receptor** by diffusion, will reside at a position of minimum free energy within the force field of that **receptor**.

For an **agonist** (or for an **antagonist**) the numerical representation of **affinity** is the reciprocal of the equilibrium dissociation constant of the ligand-**receptor** complex denoted  $K_A$ , calculated as the rate constant for offset ( $k_{-1}$ ) divided by the rate constant for onset ( $k_1$ ).

### Agonist\*\*\*

**Catabolism** consists of reactions involving endogenous organic substrates to provide chemically available energy (e.g., ATP) and/or to generate metabolic intermediates used in subsequent anabolic reactions.

### Catabolite

A catabolite is a naturally occurring metabolite.

### Clone\*

A **clone** is a population of genetically identical cells produced from a common ancestor. Sometimes, "clone" is also used for a number of recombinant DNA (deoxyribonucleic acid) molecules all carrying the same inserted sequence.

### Codon\*

A **codon** is the sequence of three consecutive nucleotides that occurs in mRNA which directs the incorporation of a specific amino acid into a protein or represents the starting or termination signals of protein synthesis.

### Coenzyme

A **coenzyme** is a dissociable, low-molecular weight, non-proteinaceous organic compound (often nucleotide) participating in enzymatic reactions as acceptor or donor of chemical groups or electrons.

### Combinatorial synthesis

**Combinatorial synthesis** is a process to prepare large sets of organic compounds by combining sets of building blocks.

### Combinatorial library

A **combinatorial library** is a set of compounds prepared by combinatorial synthesis.

### CoMFA

See Comparative Molecular Field Analysis.

### Comparative Molecular Field Analysis (CoMFA)\*\*

**Comparative molecular field analysis (CoMFA)** is a 3D-QSAR method that uses statistical correlation techniques for the analysis of the quantitative relationship between the biological activity of a set of compounds with a specified alignment, and their three-dimensional electronic and steric properties. Other properties such as hydrophobicity and hydrogen bonding can also be incorporated into the analysis. (See also Three-dimensional Quantitative Structure-Activity Relationship [3D-QSAR]).

### Computational chemistry\*\*

**Computational chemistry** is a discipline using mathematical methods for the calculation of molecular